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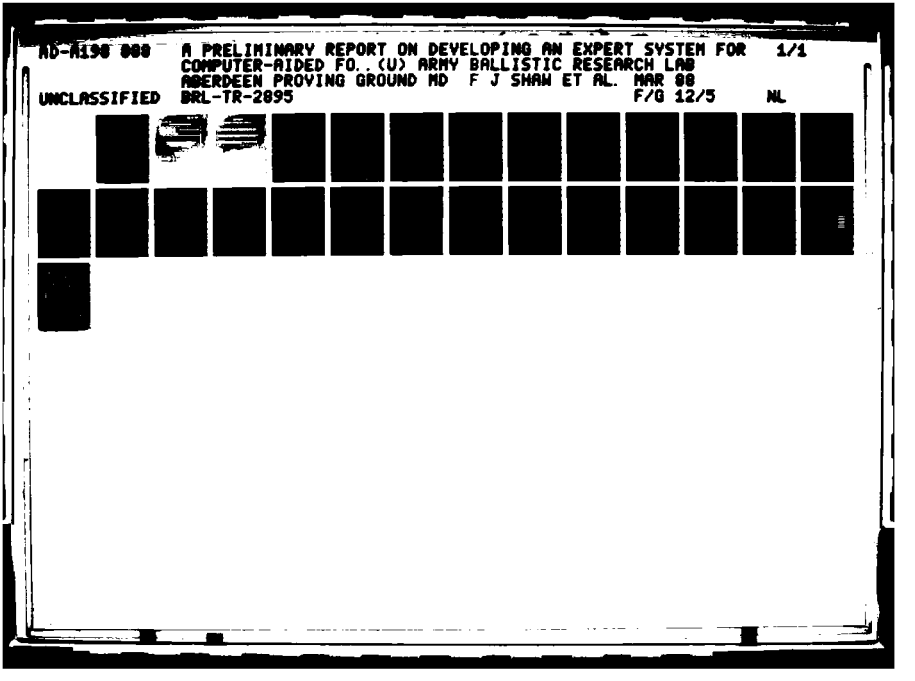

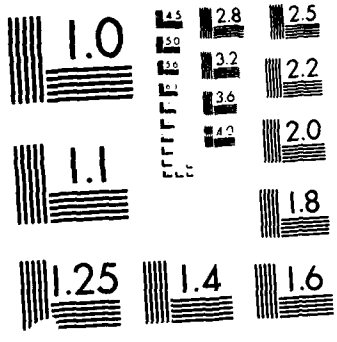

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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) BRL-TR-2895	5. MONITORING ORGANIZATION REPORT NUMBER(S)
6a. NAME OF PERFORMING ORGANIZATION US Army Ballistic Research Laboratory 6b. OFFICE SYMBOL (*If applicable*) SLCBR-IB	7a. NAME OF MONITORING ORGANIZATION
6c. ADDRESS (*City, State, and ZIP Code*) Aberdeen Proving Ground, MD 21005-5066	7b. ADDRESS (*City, State, and ZIP Code*)
8a. NAME OF FUNDING/SPONSORING ORGANIZATION 8b. OFFICE SYMBOL (*If applicable*)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
8c. ADDRESS (*City, State, and ZIP Code*)	10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO. 61102A; PROJECT NO. AH43; TASK NO.; WORK UNIT ACCESSION NO.

11. TITLE (*Include Security Classification*)

A PRELIMINARY REPORT ON DEVELOPING AN EXPERT SYSTEM FOR COMPUTER-AIDED FORMULATION OF PROPELLANTS

12. PERSONAL AUTHOR(S)

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13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (*Year, Month, Day*)	15. PAGE COUNT
Final	FROM Jan 87 TO Sep 87		26

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (*Continue on reverse if necessary and identify by block number*)
FIELD	GROUP	SUB-GROUP	
12	09		Expert System, Propellant Formulation, Expert System Shell, Insight 2+, Artificial Intelligence, Personal Computers, Propellant Formulation Properties
21	09.2		

19. ABSTRACT (*Continue on reverse if necessary and identify by block number*)

An expert system is being developed which will automate the propellant formulation design process. The expert system, being developed, uses Insight 2+, an expert system shell operating on an IBM AT-compatible microcomputer. The user is asked to specify requirements (e.g., desired energy, cost, burn rate, specific ingredient preferences) for the basic ingredients (oxidizer, binder, plasticizer,...). Based on these requirements, the individual ingredient databases are screened and those ingredients consistent with the criteria are saved to datafiles. Propellant formulations are then generated from the different possible domcinations of ingredients in the datafiles with rule-based criteria being used to exclude incompatible combinations, etc. Additional modules are being developed which will use rules, simple relationships (equations), or accessible computer programs to predict the properties (cost, sensitivity, mechanical behavior, etc.) of the formulations so generated, and interactively help the user select one or more of the formulations for a specific application.

Keywords: computer programs, solid rocket propellants (KP)

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION	
☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS	Unclassified	
22a. NAME OF RESPONSIBLE INDIVIDUAL Mr. Frederick J. Shaw	22b. TELEPHONE (*Include Area Code*) 301-278-6167	22c. OFFICE SYMBOL SLCBR-IB-I

DD Form 1473, JUN 86 *Previous editions are obsolete.* SECURITY CLASSIFICATION OF THIS PAGE

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I. INTRODUCTION

An area of Artificial Intelligence (AI) which has found increased commercial applications are expert systems. An expert system is computer software which simulates the knowledge and reasoning of a human expert. Based on information received from the user, the expert system suggests a conclusion or solution to the problem, just as a human expert would. The advantages an expert system has over a human expert are that the knowledge is permanent, and relatively easy to transfer and document; also, the conclusions given by the expert systems are consistent, and the reasoning process used to reach the conclusions can be queried and examined (not always possible with humans!). Expert systems can be used to "capture" the expertise of individuals who will not be remaining at an organization; in some cases, expert systems can combine the expertise of more than one expert, or make use of supplementary theory or data, making the expert system "smarter" than anyone of the experts that contributed to it. One major disadvantage of expert systems is the time it can take to develop a viable system. This time period can be long (months, even years).

Soon after the initial development of the first expert systems came the development of expert system software tools. These tools offer built-in capabilities such as debugging aids, input/output facilities, explanation facilities, and knowledge base editors. Expert system "shells" are one of the many different software tools available. These shells enable a programmer or "knowledge engineer" to build expert systems without using a high level AI language such as LISP, PROLOG, OPS5. The use of shells also sometimes permits non-programmers to construct expert systems; the expert himself can, in fact, do much of the expert system development, without the need of the knowledge engineer, and without the need for lengthy interviews and analysis. Also, unlike ordinary programming, an expert system constructed with a shell can be easily modified by someone other than the one who developed it, facilitating continuing improvements. Another advantage of shells is that the majority run on personal computers (pc's). Some even have versions which run on both pc's and minicomputers. Therefore, depending on the requirements of the expert system, it can be run on a pc, a minicomputer, or on both. There are also expert system shells which have been developed for running on AI-computers, i.e., minicomputers which are specifically designed for running LISP.

Expert system shells can be divided into two classes: example-based shells and rule-based shells. Example-based shells develop rules from examples entered by the knowledge engineer. For rule-based shells, the knowledge engineer enters the rules, directly. Example-based shells are easier to learn to use since all that is necessary is to enter relevant examples (e.g., formulations and the corresponding test results); there is little or no computer programming required. Developing an expert system using rule-based shells is more involved since a shell program must be written using if-then-else rules, instead of the shell developing the rules. In general, however, rule-based shells permit expert systems that are more versatile and powerful than those developed with example-based systems. An area of propellant research which should readily lend itself to the use of expert systems is the process of developing a new propellant formulation. Currently the process is more of an art than a science, i.e., the formulator has some intuitive feeling for which components to use, and the amounts, particle sizes, processing techniques, etc., to give the desired properties for a

specific application, but this design process is rarely documented. In addition, with the recent change-over from nitrocellulose to other energetic binders and especially with "inert"-binder nitramine propellants, the number of combinations of ingredients has increased by orders of magnitude. This makes it considerably more difficult to know which propellant formulation to use for a given application, and makes systematic development of "selection rules", expert systems, and other tools even more desirable than in the past. Furthermore, in addition to aiding the formulator in selecting ingredients, it should also be possible for an expert system to predict or estimate the properties of the various possible formulations as a further aid to selecting the best possible one.

II. APPROACH

We are in the process of developing an expert system for computer-aided design ("CAD") of propellant formulations. Apparently, this is the first attempt to develop an expert system for propellant formulation design; there have been a limited number of attempts to "systemize" the formulation process in ways that would be conducive to subsequent incorporation with artificial intelligence techniques,[1] but to our knowledge these efforts did not lead to an expert system approach. In other fields, however, similar goals have been successfully achieved, making us optimistic about the long term prospects for success in this endeavor. For example, computer-aided design and computer-aided manufacturing ("CAD/CAM") have been successfully applied to molecular design and engineering of chemical properties in the fields of pharmaceutical chemistry and genetic engineering. Recently, CAD techniques have been applied to the design (and selection) of polymers and composites.[2]

The expert system we are developing will aid the user in designing a propellant for an intended application, given certain user-specified constraints. The output of the expert system will be a list of possible formulations (combinations of oxidizer, binder, plasticizer, additives, etc.), as well as estimated propellant properties (energy, burning rate, sensitivity, etc.). In addition to requesting the desired propellant properties, the user will be asked to select desired criteria for the components (for example cost, a specific chemical class, inert vs. energetic). Rules will be used in selecting the components which meet the user's criteria, to screen out incompatible combinations of ingredients, and estimate the properties of the resulting formulations. Until the utility of the expert system approach for propellant formulation design and properties estimation can be demonstrated, it is probably not practical to build such an expert system for a broad class of propellants, e.g., for nitramine propellants in general. For the problem to be tractable, it is necessary at this stage to build the expert system around a narrowly-defined class of propellants, preferably from a single propellant development effort. In this way, differences in manufacturing and testing techniques will not obscure the desired rules and relationships, and (hopefully) there will be available well-documented performance test data for systematically carried out variations of formulations. Currently, we are examining the data from three experimental programs: the BRL/Rocketdyne LOVA program,[3] a related LOVA program at ARDEC,[4] and a program being carried out at NWC, China Lake.[5] These programs are all nitramine (HMX, RDX) based, and include both inert and energetic binders and plasticizers. Table 1 shows the kind of ingredient and formulation properties we will be considering as the expert system develops.

III. PROCEDURE

The expert system is being developed on a Zenith ZWX-248 AT-compatible with 640k memory and 2560k extended memory, using Insight 2+ as the expert system shell.[6] Insight 2+ is a rule-based expert system shell which uses a high level AI language called Production Rule Language (PRL). The reasoning process the shell uses is "backward-chaining", that is, the shell starts with a goal, and searches for a rule containing a premise that supports the goal. Once the rule is found, a search is made for a fact that verifies the premise. If such a fact is not found, a search is made for a rule that can be used to infer the fact or else the user is asked to supply the answer. This cycle is repeated until the goal is proved or disproved. Backward-chaining is common among expert system shells. It is usually thought of as being useful for "diagnosis" type problems, but can in fact be used for design, even though design is frequently thought of as a "forward-chaining" process.

PRL encompasses 65 keywords which include most of the mathematical functions (log, ln, sin, cos, tan). PRL also offers several features which are very desirable for developing expert systems. These include options for interfacing to external programs and searching dBASEIII+ databases, and explanation facilities for giving a more in-depth explanation of a question if requested by the user. Also the user has the option of selecting "unknown" if an answer to a question is not known. The overall structure of the language is similar to most programming languages. Variables must be declared and initialized in the beginning of the program. The rules are the if-then-else type. Expert system modules can be chained together; therefore a large expert system can be written in separate distinct modules which are then linked together. Shown below (Table 2, left) is some source code which illustrates some of the properties of PRL including variable declaration, goal definition, rules, and chaining. Also shown below (Table 2, right) is an example of a small portion of a line-of-reasoning report. (A line-of-reasoning report for a single generated formulation can be several pages in length, and will be much longer than that with properties estimation; consequently, when requested, it is written to disk and searched with a word processor.)

The procedures for interfacing to external programs and to dBASEIII+ databases are similar, since Insight 2+ uses a Pascal-based programming language ("DBPAS") to interact with dBASEIII+ databases. Shown below (Table 3, left) is a source code listing of a simple external DBPAS program (fetchbin) that "fetches" a binder from a database of binders and returns the name of the binder and three of its thirteen tabulated properties (cost, class, and inert/energetic designation) to the main program. Also shown below (Table 3, right) is a portion of a "main program" that calls this external program from within a rule, using a "call program name" statement. For accessing external programs written in a language other than DBPAS, the "activate" statement is used instead of a "call" statement. Both systems use "send" to pass data to an external program, and "return" to receive data from the external program. The external programs being accessed can be either memory-resident, or disk-resident, depending on their size and other considerations. The ability of the shell program to access external databases and programs is critical for propellant formulation design, since the propellant ingredients and their properties are initially contained in databases, and since some of the computations involved in estimating propellant properties cannot be carried out from within the rules.

Table 1. Ingredient Databases and Formulation Properties[a]

INGREDIENT DATABASES

A. Oxidizer
- name and abbreviation
- C/H/O/N, heat of formation (Hf)
- burn rate (R), impact sensitivity (Is), decomposition T (Td)
- type: nitramine, nitro, nitrate ester, ...
- particle size, density, cost

B. Binder
- name and abbreviation
- C/H/O/N, heat of formation (Hf)
- energetic (EB) or inert (IB)
- R and Is if energetic, Td
- type: ester, azido, nitro, azido-nitramine, ...
- processing types: thermoplastic (TPE), solvent (SOL), cure (CUR), cross-link (XL)
- mechanical prop.: modulus, failure stress, strain at failure
- glass transition T (Tg), density, mol. wt., cost,...

C. Plasticizer
- name and abbreviation
- C/H/O/N, heat of formation
- energetic (EP) or inert (IP)
- type: nitro, nitrate ester, nitramine, ester, ...
- impact sensitivity if energetic, Td
- melting point (Tm), boiling point (Tb), vapor P (VP)
- density, cost

D. Additives:
- name and abbreviation
- M/C/H/O/N, heat of formation, Td
- purpose: "catalyst" (CAT), stabilizer (STAB), flash suppressant (FLA), inhibitor (INH), processing aid (PRO), ...
- type: borohydride (BH), amine (AM), alkali salt (ALK), metal (M), metal hydride (MH), metal oxide (MO)
- cost, particle size

PROPELLANT PROPERTIES

A. Accurately or semi-quantitatively calculable:
- Cost, density
- Energy (impetus, specific impulse), flame temperature (Tf)
- Degree of Oxidation (e.g., O/(2(C+H)), (related to flash)

B. Estimatable:
- Burn rate, impact sensitivity (Is)
- Decomposition temperature (Td)
- Mechanical Prop.: modulus, failure stress, strain at failure
- glass transition T (Tg)

a. Tentative list: Many ingredient properties listed are not yet being used in the expert system.

Table 2. Example of PRL Source Code (Left) and Line-of-Peasoning Report (Right)

PARTIAL SOURCE CODE LISTING
OF AN INSIGHT 2+ PROGRAM

```
TITLE preliminary screening

SHARED STRING oxidizer name

SHARED SIMPLEFACT desire a specific oxidizer

SHARED NUMERIC oxidizer number

INIT oxidizer number = 1

FORGET desire a specific binder type


1.  have evaluated propellant


RULE check for completeness
IF have evaluated desired oxidizer
!AND have evaluated desired binder
!AND have evaluated desired plast
THEN have evaluated propellant
AND DISPLAY answer
AND CHAIN OXIDC
!
!OXIDIZER COST SECTION
!unlimited >250.00
RULE Can oxidizer cost be unlimited
IF select the oxidizer cost/unlimited
THEN have evaluated oxidizer cost
AND desired oxidizer cost := "unlimited"
```

LINE-OF-REASONING REPORT
Knowledge Base : binder screening

```
The following goal was pursued :
     initialized binder datafile
The program INITBIN.COM was activated.
As a result the following conclusion was reached :
     initialized binder datafile = True
The following goal was pursued :
     have evaluated binder
The program FETCHBIN was activated.
The following numeric fact was obtained :
     cost of binder = True
     Value =    150.00
The following string fact was obtained :
     binder name = True
     String = "GAP"
The following string fact was obtained :
     binder type = True
     String = "AZIDO"
The following simple fact was obtained :
     energetic binder = True
The following numeric fact was obtained :
     binder eof = True
     Value =      0.00
As a result the following conclusion was reached :
     have saved binder = True
As a result the following conclusion was reached :
     have evaluated energetic binder = True
As a result the following conclusion was reached :
     have evaluated binder cost = True
As a result the following conclusion was reached :
     have evaluated binder = True
```

The expert system is being developed and tested in separate modules. Figure 1 is a schematic representation of the operation of the various modules of the expert system. The pre-screening module (the first module) queries the user for relevant information, such as requirements and specific ingredient preferences. For example, the expert system asks the user if he wishes to use a specific oxidizer. If not, he is asked to select a maximum cost for the oxidizer (e.g., unlimited, high [<$250/lb.], medium [<$50/lb.], or low [<$10/lb.]). Answers to all questions are made by moving an arrow to the desired choice with the up/down cursor keys. During the user interrogation stage, several function keys are defined for specific purposes:

2 UNKN 3 STRT 5 EXPL 6 WHY? 8 MENU 9 HELP 10 EXIT

Function #2 UNKN(own) is selected if the user does not know the answer to a question. Pressing Function #3 will restart the program. Function #5 EXPL(anation) is available if the user needs a more detailed explanation for a question. Pressing Function #6 will display the line of reasoning the shell is pursuing at the time (i.e., a list of all the goals that are known and the rules that have been executed). Function #8 will cause a return to the

Table 3. Example of DBPAS External Program (Left) and Calling an External Program (Right)

SOURCE CODE LISTING OF A DBPAS PROGRAM

```
PROGRAM FETCHBIN

(RECEIVE INDEX : integer;

     RETURN COST : REAL;
     NAME, CLASS : STRING(25);
     ENERGETIC : BOOLEAN;
     STATUS : INTEGER);

VAR
  LAST : INTEGER;
  a : char;

BINDER : RECORD
    NAME : STRING(25);
    ABBREV : STRING(10)
    CLASS : STRING(25);
    MOL_FOR : STRING(15);
    MOL_WGHT : REAL;
    HT_OF_FORM : REAL;
    ENERGETIC : BOOLEAN;
    PROCESS : STRING(10)
    DENSITY : REAL;
    IMP_SENS : REAL;
    BURN_RATE : REAL;
    FAIL_STRESS : REAL;
    GLASS_T : REAL;
    COST : REAL;
    PARTICLE_S : REAL;
  END

BEGIN
  OPEN (BINDER, 'BINDER');
  STATUS := 1;
  last := size(BINDER);
IF INDEX <= LAST THEN BEGIN
    GOTO (INDEX, BINDER);
    STATUS :=0;
    COST := BINDER.COST;
    NAME := BINDER.NAME;
    CLASS := BINDER.CLASS;
    ENERGETIC :=BINDER.ENERGETIC;
  END
  CLOSE (BINDER);
END;
```

EXAMPLE OF ACCESSING A DBPAS PROGRAM

```
TITLE binder screening

NUMERIC cost of binder
AND binder eof

STRING binder name
AND binder type

SIMPLEFACT energetic binder
AND have evaluated binder cost
AND have evaluated binder
AND have saved binder
AND have a component
AND have evaluated binder type
AND have evaluated energetic binder
INIT binder number = 1

FORGET have evaluated binder cost
FORGET have evaluated binder
FORGET have evaluated binder type
FORGET have evaluated energetic binder
FORGET have saved binder
FORGET have a component
EXHAUSTIVE ALL
UNKNOWN CONTINUE

1. initialized binder datafile
        1.1 have evaluated binder
RULE initialize datafile
ACTIVATE INITBIN.COM
THEN initialized binder datafile

RULE Get entry from the binder database
CALL FETCHBIN
SEND binder number !record number
RETURN cost of binder
RETURN binder name
RETURN binder type
RETURN energetic binder
RETURN binder eof
IF binder eof = 0
AND have saved binder
THEN have evaluated binder
AND binder number := binder number + 1
AND CYCLE
```

program development menu. Function #9 displays a help screen of the available options. Pressing Function #10 will return control to the computer operating system (DOS). The following, for example, is what is displayed when the EXPL (Func #5) function is pressed for the question "selecting an oxidizer cost":

> "The knowledge base is requesting information on the maximum allowable oxidizer cost. This cost will be used in screening the database for candidate oxidizers. Usually, the oxidizer cost controls the materials cost of the formulation. Enter "unlimited" if you do not want cost to be a criterion."

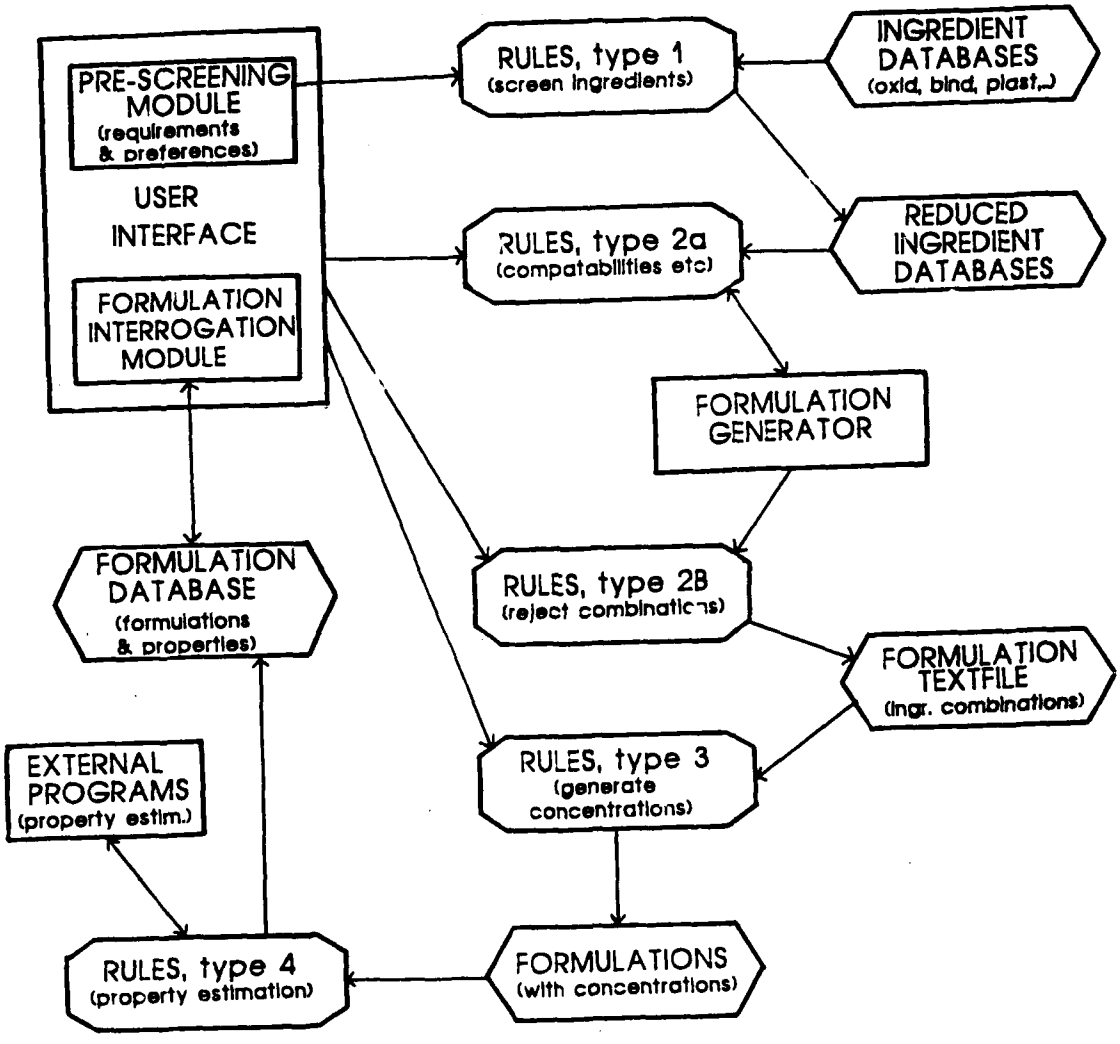

Figure 1. Flow Diagram of the Propellant Formulation Expert System. Although not shown, rules of types 2, 3, and 4 make use of properties contained in the ingredient databases.

The pre-screening module queries the user for all the necessary information, including requirements for the formulation (energy, burn rate, sensitivity, cost, etc.), and specific ingredient preferences (a specific preference for a certain ingredient, or any ingredient cost, chemical class, energetic/inert, etc., requirements).

The user-specified requirements/preferences are then used by rules (of type 1 in Figure 1), which search the individual databases (oxidizer, binder, plasticizer, ...) in series for components which meet the desired criteria. The "hits" are saved in their respective "reduced databases", or "datafiles". The next step involves the generation of ingredient combinations (one each oxidizer, binder, plasticizer) by the "formulation generator". (Mixtures of oxidizers [e.g., HMX/TAGN] or other ingredients are not allowed at the present time.) Rules control this process as well. Some of these rules (type 2a) are triggered as individual ingredients are being "fetched", and serve to reduce the number of possible combinations generated by preventing certain combinations based on considerations like known incompatibilities (e.g., if the chemical class of the oxidizer is X, and that of the binder is Y, skip [exclude] this combination). Other rules (type 2b) trigger after a combination is generated, and result in that combination being rejected. Acceptable combinations are written to a "formula textfile". The next step involves assigning concentrations to the ingredients. At the present time, we are doing this on a semiquantitative (e.g., high, medium, low) basis, values being assigned to "high", "medium", and "low" based on density and other considerations. For example, for an inert-binder/plasticizer RDX propellant, high, medium, and low for the oxidizer (RDX) concentration might be 70, 75, and 80 weight percent, respectively; for an energetic-binder or energetic-plasticizer formulation, somewhat lower values would be used. Such considerations are also taken care of by rules (of type 3 in Figure 1). The net result of assigning three concentration values to each oxidizer, binder, and plasticizer is that up to nine formulations are generated and written to the "formulations textfile" for each combination in the formula textfile.

The last two modules of the propellant formulation design expert system involve formulation properties estimation, and interrogation of the resulting formulation/properties database, as shown schematically in Figure 1. The properties estimation module is to a large extent the driving force for the expert system. Both rules (type 4 in Figure 1) and external programs are used in estimating properties for the formulations, and ingredient properties from the ingredient databases are fetched as required for use in the rules and/or external programs. Formulations with estimated properties are written to the final formulations database for subsequent interactive interrogation by the user. Examples of properties that can be evaluated within rules are cost, sensitivity, and burning rate, the first because only a simple calculation is required, the latter two because our level of understanding of the chemical interactions involved does not permit more than an approximation to be made. Energy (impetus or specific impulse) and flame temperature are examples of properties that are estimated in external programs. For properties like this, several levels of accuracy are possible: (a) a few relatively simple equations can be used to approximate (to within a few percent) the energy and flame temperature from the overall elemental composition (assuming only C/H/O/N) and heat of formation, (b) or a more exact calculation can be carried out using more detailed equations of the type that were frequently used in

"hand calculations" before computers became available,[7] (c) or, lastly, an exact calculation can be carried out by linking to a standard thermochemical code such as BLAKE or NASA-Lewis. (We are working on the first two of these methods, but expect within the near future to use the last since microcomputer versions of the thermochemical codes are now becoming available.) Examples of some simple preliminary trial equations for property estimation are as follows:

A. For burn rate (R): Rprop = Roxid * (Tfprop / Tfoxid)

Equal to R for the oxidizer times the propellant/oxidizer flame temperature ratio.

B. For glass transition temperature (Tg):

$$= Tg_{bind} - (C/MW_{plast})(X_{plast}/X_{bind})$$

where the Xs are the mass fractions of the plasticizer and binder in the propellant, and C is an coefficient obtained from published results on Tg lowering by plasticizers.

C. For decomposition temperature: Equal to the lowest of the separate ingredient decomposition temperatures.

D. For impact sensitivity (Is), (i.e., drop height in cm):

$$n = Is_{ox}/X_{ox}^{n} + X_{bind}(Is_{bind} - Is_{ox}) + X_{plast}(Is_{plast} - Is_{ox})$$

where the Xs are again the mass fractions, the Is are the impact sensitivities of the separate components (with a maximum value), and n is an integer exponent adjusted to properly represent typical dilution effects. Specific chemical interactions are not included in the above equations. However additional rules can be added to modify the results of these simple relationships for any known specific chemical interactions.

Despite the use of rules (and user requirements, preferences, etc.) to narrow down the number of ingredients being considered and to limit the number of ingredient combinations, the number of formulations in the final formulations database can be quite large. The database interrogation module in the user interface (Figure 1) aids the user in selecting formulations from this database for consideration. For example, the user can ask for a report of the 10 highest energy formulations, the 10 cheapest formulations, all formulations containing a certain ingredient or combination of ingredients, etc. Since the database is saved to disk, it can be interrogated by other users (who have the same requirements) without running the entire expert system.

IV. PRESENT STATUS OF THE EXPERT SYSTEM

At the time of writing of this report, the programming required to interrogate the user, access the dBASEIII+ ingredient databases, and generate formulations, has been completed. In accomplishing this, only a few rules of types 1-3 were included -- just enough to be sure that all of the modules worked properly together. What remains is to make this portion of the expert

system more intelligent by inserting more rules, and to develop the properties estimation module, which we are just beginning. Currently, we have only included oxidizers, binders, and plasticizers in the expert system; additives will be added after the prototype properties estimation module is completed. It is expected that the properties estimation module will evolve and grow over a long time period, being initially fairly "dumb", and eventually (hopefully!) quite "smart" as our understanding of the complex underlying inter-relationships that control certain propellant properties increases. The expert system should become immediately useful for suggesting combinations of ingredients that might not otherwise have been considered by the user, and in pointing out the knowledge gaps in our understanding of the factors that affect propellant performance. At the present time, we are relying primarily on data analysis to determine rules for compatibilities and properties, rather than on interviews with those people involved in the new formulation development programs. In doing this, we are making use of example-based expert system shell programs, such as 1st-Class.[8] As mentioned above, example-based shells do not seem versatile enough for development of an expert system of this type; they are, however, quite useful for analyzing data, uncovering relationships, and formulating rules. Typically, we might first enter the data from a test program into Lotus 1-2-3,[9] and plot the data in different ways to help point out data that does not follow normal, expected trends. For example, the properties burn rate, sensitivity and ignitability (or inverse of ignition time) might be plotted vs. computed impetus or specific impulse, in order to point out data that did not follow the normal trend of increase in the property with increasing energy. The numerical data would then be converted to a high, medium, low type format (choosing a dividing point for these ranges is a little subjective) and entered into the example-based shell along with information about the composition of the formulation. The example-based shell would then "analyze" the data and produce one or more rules that summarize the data. These rules are analyzed and then converted into a form compatible with the rule-based expert system (Insight 2+). Example-based shells that deduce rules for use in rule-based shells are apparently becoming more common: commercial products are now being introduced which directly accept data from Lotus 1-2-3 and databases, deduce rules, and convert the rules into the format required by Insight 2+ and other rule-based shells.[10]

V. DISCUSSION

Application of these techniques is relatively straightforward; the challenge lies in making the expert system really useful, and the predicted formulation properties accurate. At the present time, it is not clear how certain problems will be approached. One is that of mixed oxidizers (e.g., HMX/TAGN) and mixed binders (e.g., CAB/NC). For the time being, we will simply include these mixtures as separate entries in the respective databases; ultimately, it would be desirable for these mixtures and their properties to be generated by the expert system from the separate ingredient properties. Initially, and to make the problem more tractable, we will also be neglecting potentially significant changes in performance due to differences in particle size and processing techniques, and a number of very important properties such as burning rate exponent and temperature sensitivity coefficient. In the long term, hopefully it will be possible to have a functional group representation of the ingredients in the databases, with physical/chemical properties

predicted based on chemical structure, as has been successfully done to some extent with polymers.[2]

VI. CONCLUSION

Developing an expert system to assist in the design of propellant formulation appears to be entirely feasible, though how "intelligent" it will be, especially in estimating formulation properties, remains to be seen. However, it seems probable that any lack of intelligence in this regard will not be due to any fundamental limitations of the approach or expert system techniques, but rather to a lack of fundamental understanding of ingredient interactions and their affect on formulation properties. As such, the shortcomings should help in pointing out the knowledge gaps in our understanding of the fundamental phenomena involved, and the correlations between the properties of the individual ingredients and those of the propellant. To the extent the expert system is successful, it should help (with time) in the transformation of formulation design from an art or inefficient trial-and-error process into a rational and well-documented science.

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